CONVERSION OF UNBALANCE CHEMICAL REACTION INTO BALANCE CHEMICAL REACTION BY USING GAUSS JORDAN ELIMINATION METHOD

Deepak S Dandwate

Umesh jagannath Tupe
Vidya-Amrut Dnyan Pratisthan’s Arts,Science and Commerce College, Shirsondi T…

Original Research Paper | Computer Science | Volume : 6 ¦ Issue : 1 ¦ Jan 2021 ¦ e-ISSN : 2456-5040

CONVERSION OF UNBALANCE CHEMICAL REACTION INTO BALANCE CHEMICAL REACTION BY USING GAUSS JORDAN ELIMINATION METHOD

***Madhuri A. Gaikwad [1], Sapna V. Walekar[1], Chetna A. Desale[1], Deepak S. Dandwate [1], Umesh J. Tupe [1], Sonali V. Walekar[2]**

[1]M. G. Vs, Department of Computer Science, Panchavati College of Management & Computer Science, Nashik, India. (*Corresponding Author)
[2]Department of Computer Science, VCACS College, Pune, India.

ABSTRACT

Rapid changes in technology have made the valuable overview on the application of matrices relevant not just to mathematicians, but to abroad range of other fields. A relationship between mathematics and chemistry is so familiar that a certain amount is balanced or maintained when a chemical reaction occurs. In chemical reactions balancing equations is very basic and fundamental concept. In some cases it becomes more difficult to solve. So that a mathematical treatment is more useful in order to make it simple. This research paper mainly focuses on an excellent application of Gauss-Jordan elimination method for balancing chemical equations. The result shows that, in first example 4 atoms of sodium (Na), 12 atoms of oxygen (O), 8 atoms of Hydrogen (H), and 2 atom of sulfur (S) are same each on both the reactants and products makes the chemical equation balance. This result satisfies the law of conservation of matter and confirms that there is no contradiction in the existing way of balancing chemical equations.

KEYWORDS: Matrix, Homogeneous linear equation, Balanced chemical equation, unbalanced chemical equation.

INTRODUCTION:C

Matrices have a long history of applications in solving linear equations, between 300BC and AD200. The term matrix was coined by Sylvester, Who understood a matrix as an object giving rise to number of determinants today is called as minors. The first concept of mathematics was applied around 1850 AD but its application was applicable in ancient times. The Latin word matrix means worm. It means anything that is usually made or created anywhere. He demonstrated the first significant use of the notation A=aij to represent a matrix where aij is an element in the i^{th} row and the j^{th} column. Matrices can be used to solve the system of linear equations simultaneously [4].

A matrix is represented in the form of a rectangular block that contains a number of rows and columns. Items in the matrix are called elements or entries. The size or order of matrix is m x n where m is the number of rows and n is the number of columns of the matrix. If the order of matrices are same then we can add or subtract matrices in element wise .Multiplication of two matrices are possible if the number of columns of first matrix is equal to the number of rows of second matrix. Scalar multiplication of matrix is nothing but a scalar is multiply by each & every entry of the matrix [1]. In chemistry, Willian C. Herndon [2] in his research article presented number of papers on balancing chemical equation which is most useful to research. Also he proposed comparative methods in balancing chemical reaction equations. In research discussion, Ice B. Risteski [3] applied a new singular matrix method in chemical equation balancing and used the theory of solving homogenous equations by Drazin pseudo matrix. Also he proposed comparative methods in balancing chemical reaction equations. In research discussion, Ice B. Risteski applied a new singular matrix method in chemical equation balancing and used the theory of solving homogenous equations by Drazin pseudo matrix.

APPLICATION OF MATRIX:

In the computing field, matrices are used in message encryption. Also matrix is used to create three-dimensional graphic images and realistic looking motion in the calculation of algorithms that create Google page rankings & also in a two-dimensional computer screen. Some of the application of the matrix as follows.

1. **Cryptography:** The most important component of the Hill Cypher is the key matrix. The key matrix is useful for an encrypt the messages, and its inverse to decrypt the encoded messages. It is important that the role of key matrix is kept secret between the message senders and intended recipients. If the key matrix or its inverse is finding, then all intercepted messages can be easily decoded. However, you cannot use just any matrix as a key. First, the matrix must be invertible, which means that its determinant cannot be zero [5].

2. **Computer Graphics:** Before architecture, cartoons and automation were done with hand drawings, but today they are done using computer graphics. In the video game industry, matrices are an important mathematical tool for manipulate and construct a realistic animation of a polygonal figure. Computer graphics software is a process in which linear transformations converted into translate images with the help of matrices. With the help of matrix t three dimensional images converted into dimensional planes projection.

3. **Economics:** Cramer's Rule and determinants of matrix are simple and important tools for solving many problems in business and economics related to maximize profit and minimize loss. Variance and covariance are finding with the help of matrix. The equilibrium of markets in IS-LM model is solved by using determinants and Matrix Cramer's Rule.

4. **Financial Records:** Matrices are representing array of many numbers as a single object and it is denoted by a single symbol then calculations are performed on these symbols in very compressed form. The matrix method is used in opening and closing balances for any accounting period is very less time consuming, accurate and efficient.

5. **Physics:** Matrices are used in science of optics to account for reflection and for refraction. Also it is used in electrical circuits, quantum mechanics and resistor value conversion of electrical energy. In electric circuits matrices are used to solve AC network equations and find the values of electrical parameters such as current, power and voltage [6].

Linear equation:

Linear equations are equations of the first order. In the coordinate system linear equations are defined for lines .Straight line equation is called a linear equation. y=mx+b be the general form of linear equation, where m be the slope of the line and b is the y-intercept [1].

Linear equation has two types:

1. Homogenous linear equation
2. Non-Homogeneous equation

FORMING HOMOGENOUS LINEAR EQUATIONS:

For balancing chemical reaction equations, matrix algebra are useful. Chemical reaction equations can be solving with the help of chemical equation balancing techniques which is so innovative & interesting. There are a number of balancing techniques provided by researchers so far, but the following method is completely different from previous methods.

Perquisites:

1) Every chemical reaction can be represented by homogeneous linear equation AX =0 where A be the reaction matrix and X be the column matrix of coefficients of elements and 0 be the null column matrix.

2) Chemical reaction is called as feasible reaction, if the homogeneous linear equation AX =0 has non trivial solution.

3) Chemical reaction is called as infeasible reaction, if the homogeneous linear equation AX =0 has only trivial solution [7].

METHODOLOGY:

In this section, the linear algebra method is used to balance chemical equations for its equilibrium condition. Chemical equations balanced here appears in many chemistry books and Guassian elimination method giving us an upper triangular matrix or Echelon matrix of matrix algebra for the purpose of balancing chemical equations.

Below examples are showing the balancing technique by using the Gauss-Jordan elimination method.

Example: 1

The reactants are sodium hydroxide $(NaOH)$ and sulfuric acid (H_2SO_4) then the Products sodium sulfate (Na_2SO_4) and water (H_2O) get when they react & its chemical equation representation is as below

The chemical reaction is:

$$2NaOH\ +\ 2H_2SO_4\ \rightarrow\ Na_2SO_4\ +\ H_2O \qquad [Not\ Balanced]$$

Put the unknowns, to balance this chemical equation then multiplying the reactants and the products to get an equation of the form.

$$x(2NaOH) + y(\ 2H_2SO_4)\ \rightarrow\ z(\ Na_2SO_4)\ +\ w(H_2O)$$

Next, we compare the no. of sodium (Na), oxygen (O), hydrogen (H), and sulphur (S) atoms of the reactants with the no. of the products. Then, four linear equation we getting.

$$Na:\quad 2x = 2z$$

$$O:\quad 2x + 8y = 4z + w$$

$$H:\quad 2x + 4y = 2w$$

$$S:\quad 2y = z$$

This is important to note that we made use of the subscripts because they count the number of atoms of a particular element .Rewrite these equations in standard format then we observe that we have a homogenous linear system in four unknowns, that is, x, y, z & w.

$$2x\ +\ 0y - 2z\ +\ 0w = 0$$

$$2x\ +\ 8y - 4z - w\ =\ 0$$

$$2x\ +\ 4y\ +\ 0z - 2w\ =\ 0$$

$$0x\ +\ 2y - z\ +\ 0w\ =\ 0$$

Alternatively;

$$2x - 2z\ =\ 0$$

$$2x\ +\ 8y\ - 4z - w\ =\ 0$$

$$2x\ +\ 4y - 2w\ =\ 0$$

$$2y - z\ =\ 0$$

We represent the above system of homogeneous linear equations in matrix form

Solving above system of linear equation by using Gauss Jordan elimination method or Reduced row echelon form method. Now we use here row operation.

$$\left[\begin{array}{cccc|c} 2 & 0 & -2 & 0 & 0 \\ 2 & 8 & -4 & -1 & 0 \\ 2 & 4 & 0 & -2 & 0 \\ 0 & 2 & -1 & 0 & 0 \end{array}\right]$$

$$\left(\frac{1}{2}\right) R_1 \sim$$

$$\left[\begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 2 & 8 & -4 & -1 & 0 \\ 2 & 4 & 0 & -2 & 0 \\ 0 & 2 & -1 & 0 & 0 \end{array}\right]$$

$R_2 - 2\,R_1,\ R_3 - 2\,R_1 \sim$

$$\left[\begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 0 & 8 & -2 & -1 & 0 \\ 0 & 4 & 2 & -2 & 0 \\ 0 & 2 & -1 & 0 & 0 \end{array}\right]$$

$\left(\frac{1}{8}\right) R_2 \sim$

$$\left[\begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & -1/4 & -1/8 & 0 \\ 0 & 4 & 2 & -2 & 0 \\ 0 & 2 & -1 & 0 & 0 \end{array}\right]$$

$R_3 - 4R_2, \quad R_4 - 2\,R_2 \sim$

$$\left[\begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & -1/4 & -1/8 & 0 \\ 0 & 0 & 3 & -3/2 & 0 \\ 0 & 0 & -1/2 & 1/4 & 0 \end{array}\right]$$

$\left(\frac{1}{3}\right) R_3 \sim$

$$\left[\begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & -1/4 & -1/8 & 0 \\ 0 & 0 & 1 & -1/2 & 0 \\ 0 & 0 & -1/2 & 1/4 & 0 \end{array}\right]$$

$R_4 + \frac{1}{2} R_3 \sim$

$$\left[\begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & -1/4 & -1/8 & 0 \\ 0 & 0 & 1 & -1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{array}\right]$$

$R_1 + R_3,\ R_2 + \frac{1}{4} R_3 \sim$

$$\left[\begin{array}{cccc|c} 1 & 0 & 0 & -1/2 & 0 \\ 0 & 1 & 0 & -1/4 & 0 \\ 0 & 0 & 1 & -1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{array}\right]$$

Now we write equation from the above matrix

$$x - \frac{1}{2}w = 0 \qquad ---(1)$$

$$y - \frac{1}{4}w = 0 \qquad ----(2)$$

$$z - \frac{1}{2}w = 0 \qquad ----(3)$$

Now we solve the above equations for x, y, z & w, we get

$$\therefore \quad x = \frac{1}{2}w \qquad --- From\ eq^n\ (1)$$

$$\therefore \quad y = \frac{1}{4}w \qquad --- From\ eq^n\ (2)$$

$$\therefore \quad z = \frac{1}{2}w \qquad -- From\ eq^n\ (3)$$

we observe that all entries are zero of the fourth row of matrix (A) ,therefore we conclude that w be a free variable. So, we can choose $w = 4$, then the values of x, y, z are

$$x = 2, y = 1, z = 2, w = 4.$$

Now ,in this case our balance chemical equation is,

$$2(2NaOH) + 1(2H_2SO_4) \rightarrow 2(Na_2SO_4) + 4(H_2O)$$

$$4NaOH + 2H_2SO_4 \rightarrow 2Na_2SO_4 + 4H_2O \qquad \text{[Balanced]} \quad [8]$$

Example: 2

Consider unbalance chemical equation

$$CH_4 + O_2 \rightarrow CO_2 + H_2O \qquad ----- [Not\ Balance]$$

The reactants are Methane (CH_4) and Oxygen (O_2) then the Products are Carbon dioxide (CO_2) and water (H_2O) get when they react & its chemical equation representation is as below

The chemical reaction is:

$$x(CH_4) + y(O_2) \rightarrow z(CO_2) + w(H_2O)$$

Next, we compare the no. of Carbon (C), Hydrogen (H) and Oxygen (O) atoms of the reactants with the no. of the products. Then We get four linear equation.

$$C: \quad x = z$$

$$H: \quad 4x = 2w$$

$$O: \quad 2y = 2z + w$$

This is important to note that we made use of the subscripts because they count the number of atoms of a particular element .Rewrite these equations in standard format then we observe that we have a homogenous linear system in four unknowns, that is, x, y, z & w.

$$x + 0y - z + 0w = 0$$

$$4x + 0y + 0z - 2w = 0$$

$$0x + 2y - 2z - w = 0$$

Alternatively;

$$x - z = 0$$

$$4x - 2w = 0$$

$$2y - 2z - w = 0$$

We represent the above system of homogeneous linear equations in matrix form

Solving above system of linear equation by using Gauss Jordan elimination method or Reduced row echelon form method .Now we use here row operation.

$$\left[\begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 4 & 0 & 0 & -2 & 0 \\ 0 & 2 & -2 & -1 & 0 \end{array}\right]$$

$R_2 - 4R_1 \sim$

$$\left[\begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 4 & -2 & 0 \\ 0 & 2 & -2 & -1 & 0 \end{array}\right]$$

$\frac{1}{2}R_3\sim$

$$\left[\begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 4 & -2 & 0 \\ 0 & 1 & -1 & -1/2 & 0 \end{array}\right]$$

$R_{23}\sim$

$$\left[\begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & -1 & -1/2 & 0 \\ 0 & 0 & 4 & -2 & 0 \end{array}\right]$$

$\frac{1}{4}R_3\sim$

$$\left[\begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & -1 & -1/2 & 0 \\ 0 & 0 & 1 & -1/2 & 0 \end{array}\right]$$

$R_1 + R_3\,, R_2 + R_3\sim$

$$\left[\begin{array}{cccc|c} 1 & 0 & 0 & -1/2 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1/2 & 0 \end{array}\right]$$

Now we write equation from the above matrix

$$x - \frac{1}{2}w = 0 \qquad ----(1)$$

$$y - w = 0 \qquad ----(2)$$

$$z - \frac{1}{2}w = 0 \qquad ----(3)$$

Now we solve the above equations for x, y, z & w, we get

$$\therefore \quad x = \frac{1}{2}w \qquad ---\ From\ eq^n\ (1)$$

$$\therefore \quad y = w \qquad ---\ From\ eq^n\ (2)$$

$$\therefore \quad z = \frac{1}{2}w \qquad --\ From\ eq^n\ (3)$$

we observe that all entries are zero of the fourth row of matrix (A) ,therefore we conclude that w be a free variable. So, we can choose $w = 2$, then the values of x, y, z are

$$x = 1, y = 2, z = 1, w = 2.$$

Now ,in this case our balance chemical equation is,

$$1(CH_4) + 2(O_2) \rightarrow 1(CO_2) + 2(H_2O)$$

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \qquad -----[\,Balance]\ [9]$$

CONCLUSION:

This allows the average and even the least accomplished students a real chance of success. It can often remove what it is a source of frustration and failure that keeps students away from chemistry. Also, it allows high achievers. Even relatively difficult equations become faster and more accurate. A balancing technique based on augmented-matrix protocols was described in this paper. Due to its unusual nature, it was best described through demonstrations in procedures. The practical superiority of the matrix process as the most common tool for balancing chemical equations is visible. So, we conclude that the mathematical method given here applies to all possible cases of balancing the chemical equation.

ACKNOWLEDGEMENT:

We are very much thankful to M.G. V's Panchavati College of Management & Computer Science, Nashik for providing lab facility with computer and internet, I would also thanks to Principal and Computer Science, Head of the Department of our college, for his constant guidance and extensive support to encourage for this work.

REFERENCES:

I. Camp, D. R. (1985). Secret codes with matrices. Mathematics Teacher, 78(9), 676–680. Lee, P. Y. (2005).

II. William, C. Herndon. On Balancing Chemical Equations: Past and Present, J. Chem. Educ., 1997,74(11), 1359, DOI:10.1021/ed074p1359.

III. Risteski, Ice B. A New Singular Matrix Methodfor Balancing Chemical Equations and Their Stability, Journal of the Chinese Chemical Society, 2009, 56, 65-79

IV. Aparna, M. "APPLICATIONS OF MATRIX MATHEMATICS." (2016).

V. Beauregard, Raymond A.; Fraleigh, John B. (1973), A First Course In Linear Algebra: with Optional Introduction to Groups, Rings, and Fields, Boston: Houghton Mifflin Co., ISBN 0-395- 14017-X

VI. E. Ulrychova; Several real world applications of Linear Algebra Tools.

VII. Krishna, Y. Hari, N. Vijaya, and P. Bindu. "Balancing chemical equations using Gauss-Jordan Elimination aided by MATLAB."

VIII. Gabriel, Cephas Iko-ojo, and Gerald Ikechukwu Onwuka. "Balancing of chemical equations using matrix algebra." *Journal of Natural Sciences Research* 3 (2015): 29-36.

IX. Clugston, M., Flemming, R. (2002). Advanced Chemistry. Oxford University press.

X. Guo, C. (1997): *Journal of Chemical Education 74*: 1365.